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Non-local ocean mixing model and a new plume model for deep convection

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Abstract

Turbulent fluxes can be represented by a diffusivity tensor, the symmetric part of which describes "*turbulent diffusion*" while the anti-symmetric part describes "*advection*". Diffusion is a local process in the sense that it depends only on the local gradients of the mean fields while advection is non-local for it is represented by an integral over all length scales (all eddies) that can "fit" from say the bottom of the physical domain to the z where the fluxes are computed.

In the ocean, there are two main regimes where non-local transport is important. One regime is where storms release a sudden burst of mechanical energy to the ocean surface that is then transported downward by energetic eddies that deepen the mixed layer. Even relatively simple non-local models yield results considerably more realistic than those of local models. The second regime is deep convection (DC) caused by loss of surface buoyancy, the description of which is required for a reliable assessment of water masses formation.

At present, there is no reliable model for either of these non-local regimes individually or much less a formalism capable of accounting for both regimes simultaneously. The goal of this paper is to present a formalism that provides the expressions for the non-local fluxes for momentum, heat and salinity encompassing both cases. Since the resulting number of dynamic equations involves is however large, we work out two sub-models, one when only shear must be treated non-locally (e.g., when storms release mechanical energy) and one when only buoyancy is to be treated non-locally (the DC case).

We employ the Reynolds Stress formalism in which non-locality is represented by the third-order moments which in turn depend on the fourth-order moments for which we employ a new model that has been tested against LES data, aircraft data and a full PBL simulation.

For the DC case, we rewrite the non-local model in terms of Plumes since thus far the only non-local model used to treat oceanic DC has been the "plume model" of Morton, Taylor and Turner (MTT model). We show that the MTT model has two key limitations, (1) an important physical process such as the rate of entrainment cannot be determined by the model and remains an adjustable parameter and (2) MTT is purely advective and thus only applicable to the initial stages of DC but not to the whole process which is both advective and diffusive. The model we derive bypasses these limitations, is a generalization of the MTT model and is applicable to the entire development of deep convection.
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1. Local models. Brief summary

In previous papers (Canuto et al., 2001, 2002, 2004a,b; cited as C1,2,4a,b), the authors presented the most complete local mixing model that present knowledge of the Reynolds Stress Model allowed us to construct. The model has essentially no adjustable parameters and includes temperature, salinity (double-diffusion), and velocity fields. In the stationary and local case, the dynamic equations for the Reynolds stresses, heat flux, salinity flux, temperature variance, salinity variance and temperature–salinity correlations, were solved analytically. The resulting momentum, heat and salinity fluxes were found to have the forms:

$$\overline{uw} = -K_m \frac{\partial U}{\partial z}, \quad \overline{vw} = -K_m \frac{\partial V}{\partial z}, \quad \overline{w\theta} = -K_h \frac{\partial T}{\partial z}, \quad \overline{ws} = -K_s \frac{\partial S}{\partial z} \tag{1a}$$

Here, overbars indicate a time or ensemble average, u, v, w, θ, s are the fluctuating components of the velocity, temperature and salinity fields whose mean components are U, V, T, S, and the K_α's are the momentum, heat and salt diffusivities. Furthermore, the mass flux is given by:

$$\overline{\rho w} = -K_\rho \frac{\partial \overline{\rho}}{\partial z} = g^{-1}\rho_o K_\rho N^2, \quad K_\rho = (K_h - R_\rho K_s)(1 - R_\rho)^{-1} \tag{1b}$$

Here, K_ρ is the mass diffusivity given in terms of the heat and salt diffusivities, N is the Brunt–Vaisala frequency, R_ρ is the density ratio $R_\rho = (\alpha_S \partial S/\partial z)(\alpha_T \partial T/\partial z)^{-1}$, where $\alpha_{T,S}$ are the thermal expansion and haline contraction coefficients. The diffusivities K_α were derived to have the following form:

$$K_\alpha = \Gamma_\alpha \frac{\varepsilon}{N^2}, \quad \Gamma_\alpha = \frac{1}{2}(\tau\Sigma)^2 Ri S_\alpha(Ri, R_\rho) \tag{1c}$$

where $Ri = N^2\Sigma^{-2}$ is the Richardson number, $\Sigma = (U_z^2 + V_z^2)^{1/2}$ is the mean shear, $\tau = 2\,K/\varepsilon$ is the eddy's dynamical time scale, K is the turbulent kinetic energy and ε is the rate of dissipation of K. Finally, $S_\alpha(Ri, R_\rho)$ are algebraic dimensionless structure functions given in C2 (Eqs. (13)–(15)). The Γ_α are called *mixing efficiencies* and most past models have assumed that there is only one Γ with a value of 0.2 (Osborn, 1980). By contrast, the C1,2 models compute the Γ_α (C2, Fig. 7). To give a concrete example of how the model is used, consider the total production of turbulent kinetic energy P, defined as the sum of shear and buoyancy contributions, $P = P_s + P_b$ where:

$$P_s = -(\overline{uw}U_z + \overline{vw}V_z) = K_m\Sigma^2, \quad P_b = -g\rho_0^{-1}\overline{\rho w} = -K_\rho N^2 \tag{2a}$$

Substituting the above results into the production = dissipation relation, $P = \varepsilon$, one obtains after simple algebra:

$$\frac{1}{2}(\tau\Sigma)^2(S_m - Ri S_\rho) = 1 \tag{2b}$$

Using the algebraic forms of the functions S_α derived in C2, Eq. (2b) yields $\tau\Sigma$ in terms of Ri, R_ρ. The mixing efficiencies $\Gamma_\alpha(Ri, R_\rho)$ are then obtained from Eq. (1c) and are exhibited in Fig. 7 of C2. Finally, the diffusivities are computed from (1c) after one specifies the physical processes responsible for the dissipation ε, a topic we discuss next.

1.1. Mixed layer. Shear instabilities

In the mixed layer where shear instabilities dominate, the dissipation is computed as ($\varepsilon = K^{3/2}\Lambda^{-1}, \tau = 2K/\varepsilon$):

$$\varepsilon_{\mathrm{ML}} = 8\Lambda^2\Sigma^3(\tau\Sigma)^{-3} \tag{2c}$$

where Λ is a mixing length discussed in C2 (their Eqs. (24a,b)).

1.2. Abyssal ocean. Internal gravity waves (IGW)

In the thermocline, where internal gravity waves contribute the most to the dissipation and thus to the diffusivities, we used for ε the expression suggested by the Gregg–Henyey–Polzin model (Polzin et al., 1995; Polzin, 1996; Kunze and Sanford, 1996; Gregg et al., 1996; Toole, 1998):

$$\varepsilon_{\mathrm{IGW}} = 0.288N^2L(\theta, N) \tag{2d}$$

where the latitude dependence factor $L(\theta, N)$ has been given by Gregg et al. (2003). The implications of (2d) on the sharpness of the equatorial thermocline have been recently studied in C4b.

Finally, in C1,2 the results of the new mixing models were assessed using the z-coordinate NCAR ocean stand alone code. Several global and local results were discussed vs. Levitus data and the NATRE experiment (Ledwell et al., 1993, 1998).

2. Non-locality. Physical considerations

As Eq. (1a) shows, the C1,2 is a local model since the fluxes at z are computed using the gradients of the mean fields at the same location. On the other hand, there are physical reasons to believe that a local model is incomplete since *turbulence not only produces non-zero correlations such as the ones in Eq. (1a), but also transports them, a feature that local models do not encompass.* Non-locality means that in regions where there is no local production of turbulence, mixing is nonetheless present since it was produced elsewhere and transported there by non-local effects. To quantify the argument, consider the heat flux $J_h = \overline{w\theta}$. A general expression that exhibits non-locality is of the form:

$$J_h(z) = \int^z G(z, z')\frac{\partial T}{\partial z'}\,\mathrm{d}z' \tag{3a}$$

where $G(z, z')$ has the dimension of a heat diffusivity divided by a length. Clearly, the heat flux at z is given by the contribution of all the fluxes up to z and in that sense Eq. (3a) is a very general expression for a non-local flux.

To show that a turbulence model that accounts for the third-order moments gives rise to the same expression as (3a), we consider the formal solution of the second-order moments in which the third-order moments were left unchanged. Such a solution was found by Canuto et al. (2005a) and reads as follows:

$$J_h = -K_h\frac{\partial T}{\partial z} + A_1\frac{\partial \overline{w^3}}{\partial z} - A_2\frac{\partial \overline{w\theta^2}}{\partial z} - A_3\frac{\partial \overline{w^2\theta}}{\partial z} \tag{3b}$$

The first term represents the local model while the remaining three terms represent non-locality. The functions K_h and $A_{1,2,3}$ (the A_k's do not have the units of diffusivity) were found to be:

$$DK_h = 2K\tau, \quad DA_1 = \frac{9\tau^2}{50}\frac{\partial T}{\partial z}, \quad DA_2 = \frac{3}{5}g\alpha\tau^2, \quad DA_3 = 3\tau \tag{3c}$$

where $D = 36 + 1.8N^2\tau^2$, $N^2 = g\alpha\partial T/\partial z$. Below in section VI we show that the stationary solution of the dynamic equations for the third-order moments are given by Eqs. (14a)–(14d) or even more simply by Eq. (14e). Substituting the latter into (3b) and assuming $J_{zz} \approx 0$ (which is valid in the well-mixed steady state PBL), we obtain:

$$J_h = J_\ell + \ell_*\frac{\partial J_h}{\partial z} \tag{3d}$$

where

$$J_\ell = -K_h\frac{\partial T}{\partial z} \tag{3e}$$

is the local flux while the non-local contribution is given by the second term in (3d) where the length ℓ_* is given by:

$$D\ell_* = -10^{-2}\tau^2N^2\frac{\partial\tau^2\overline{w^2}}{\partial z} + \tau\frac{\partial\tau\overline{w^2}}{\partial z} + \frac{3}{5}g\alpha\tau^2\frac{\partial\tau J_h}{\partial z} \tag{3f}$$

and is expressed in terms of only second order moments. A simple way to solve (3d) is by approximating the heat flux J_h that appears in the last term in (3f) with J_ℓ given by (3e). At which point, Eq. (3d) becomes a first-order differential equation that can be solved analytically with the result:

$$J_h(z) = \int^z dz' G(z,z') \frac{\partial T}{\partial z'} \tag{3g}$$

$$G(z,z') = \exp[\alpha(z') - \alpha(z)] K_h(z') \ell_*^{-1}(z') \tag{3h}$$

$$\alpha(z) = -\int^z \frac{dz'}{\ell_*(z')} \tag{3i}$$

Eq. (3g) has indeed the structure (3a).

3. Non-locality. Past models

Here, we briefly review past non-local models. In the case of the planetary boundary layer PBL, several authors have suggested *semi-empirical non-local models* for the heat and scalar fluxes by adding to the local terms heuristic non-local terms, also known as counter-gradient terms (Deardorff, 1972; Troen and Mahrt, 1986; Holtslag et al., 1990, 1991, 1993; Wyngaard and Weil, 1991). For a convective PBL, Holtslag and Moeng (1991) have suggested the expression:

$$J_h = -K_h \frac{\partial T}{\partial z} + \Gamma_h, \quad \Gamma_h = 0.1 w_* h^{-1} \tau \overline{w\theta}|_{\text{surf}} \tag{4}$$

where $w_* = (g\alpha h \overline{w\theta}|_{\text{surf}})^{1/3}$. As one can notice, (4) is a simplified form of the fourth term in (3b). In spite of these simplifications, Holtslag and Boville (1993) showed that this non-local model transported moisture more efficiently from the surface to higher vertical levels in a global climate model. In the ocean case, Large et al. (1994) adopted the non-local model of Troen and Mahrt (1986) for the heat flux which is also of the form (4).

However, several questions remain unanswered. Consider the salinity flux. Does it behave like the temperature flux? Are the coefficients in the PBL non-local model the same as in the ocean? Why only the heat/salinity flux? Why not the momentum flux as well? Regrettably, we cannot answer most of these questions since a general non-local model does not yet exist.

One could argue that only the temperature/salinity fields must be treated non-locally and that is the underlying assumption of the work of Large et al. (1994). Since the Labrador Sea, Gulf of Lyon and the Weddell Sea are the seats of buoyancy-dominated mixing (Deep Convection, DC), one must treat those processes non-locally since the eddies that are involved are as large as they can be and for such a case a local model is certainly inadequate. In the Large et al., model, the non-locality is activated only when there are surface losses of buoyancy that render the surface waters quite dense and thus prone to sinking. The non-local DC regions are quite limited in geographic extent since most of the world's ocean mixing is not driven by DC but by shear. Should the momentum flux be treated locally or non-locally? We face here a problem of completeness: if we want to treat non-locality without prejudging which field is affected and which is not, we must treat all three fields T, S, $\mathbf{U}$ as non-local. This is borne out by recent simulations vs. data comparison studies (Ferrero and Racca, 2004; Ferrero, 2005; Ferrero and Colonna, in press) which show that in the pure shear case:

$$\text{pure shear case}: \ \overline{u^2 w} \sim \overline{v^2 w} \sim \overline{w^3} \sim S_w \tag{5a}$$

while in the shear and convection case the third-order moments:

$$g\alpha\tau\overline{w^2\theta}, \quad \overline{w^3}, \quad (g\alpha\tau)^2\overline{w\theta^2} \tag{5b}$$

contribute to the dynamic equations with similar weight. In treating all fields as non-local, we face however two problems. First, a heuristic approach is out of the question because it would entail a myriad of adjustable parameters even admitting that one knew how to write the phenomenological expressions for all the fluxes. Second, the only alternative is to rely on the dynamic equations that describe the third-order moments but those equations entail fourth-order moments (FOMs) which have traditionally been the weakest point in any turbulence-based approach to mixing. A key priority is to construct a reliable model for the FOMs, a topic that we presented in detail in Cheng et al. (2005) and which we summarize for completeness in Appendix C.

4. Non-local models with shear and buoyancy

Let us consider the four dynamic equations for the mean velocity, temperature and salinity fields:

$$\frac{DU}{Dt} = -\frac{\partial \overline{uw}}{\partial z}, \quad \frac{DV}{Dt} = -\frac{\partial \overline{vw}}{\partial z} \tag{5c}$$

$$\frac{DT}{Dt} = -\frac{\partial \overline{w\theta}}{\partial z}, \quad \frac{DS}{Dt} = -\frac{\partial \overline{ws}}{\partial z} \tag{5d}$$

where for simplicity we have left out external sources. As one can observe, one needs four second-order moments, $\overline{uw}$, $\overline{vw}$, $\overline{w\theta}$, $\overline{ws}$. However, it turns out that their dynamic equations involve other second-order moments so that in practice one needs the dynamic equations for the following variables:

$$\begin{aligned}
&\text{Velocity field}: \ \overline{uw}, \overline{vw}, \overline{uv}, \overline{u^2}, \overline{w^2}, K \\
&\text{Temperature field}: \ \overline{w\theta}, \overline{u\theta}, \overline{v\theta}, \overline{\theta^2} \\
&\text{Salinity field}: \ \overline{ws}, \overline{us}, \overline{vs}, \overline{s^2} \\
&\text{Temperature–salinity correlation}: \ \overline{s\theta} \\
&\text{Dissipation}: \ \varepsilon
\end{aligned} \tag{6}$$

With the turbulent kinetic energy K and the dissipation ε one then constructs the dynamical time scale $\tau = 2K/\varepsilon$ that enters in all dynamic equations. Finally, since turbulence is not isotropic and $K = \frac{1}{2}(\overline{u^2} + \overline{v^2} + \overline{w^2})$, one needs K, $\overline{u^2}$ and $\overline{w^2}$. To avoid interrupting the presentation, we give the full set of dynamic equations for the variables (6) in Appendices A–C.

The complete non-local model entails 15 time dependent differential equations for the second order moments and 16 time dependent differential for the third-order moments for the temperature field. The salinity will require an analogous set of equations which can be obtained from the previous ones using symmetry arguments based on Eq. (11b). In what follows, we present two simpler non-local models which represent a good approximation to the full model. We shall divide the ocean into shear-driven, non-convective regimes and convectively driven regimes.

5. Shear driven regimes

In a stably stratified ocean, most of the mixing is shear driven. We consider the fluxes of temperature and salinity to be local since these terms are sinks in the budget for K while the velocity field is treated non-locally since it acts like a source and thus its tendency is to give rise to large eddies. Specifically, Eqs. (2)–(4) of Appendix A are taken to be local. This allows us to solve them analytically with the following results:

$$\overline{w\theta} = -K_h \frac{\partial T}{\partial z}, \quad \overline{ws} = -K_s \frac{\partial S}{\partial z} \tag{7}$$

where the heat and salt diffusivities are given by:

$$\Delta_h K_h = \pi_4 \tau \left[\overline{w^2} - \pi_2 (1-\gamma_1) g \alpha_s \tau \overline{ws} - \frac{1}{4} \alpha_3 \pi_4 \tau (\overline{uw} U_z + \overline{vw} V_z) \right] \tag{8}$$

$$\Delta_s K_s = \pi_1 \tau \left[\overline{w^2} + \pi_2 (1-\gamma_1) g \alpha_T \tau \overline{w\theta} - \frac{1}{4} \alpha_3 \pi_1 \tau (\overline{uw} U_z + \overline{vw} V_z) \right] \tag{9}$$

while the dimensionless functions $\Delta_{h,s}$ are given by:

$$\Delta_h = 1 + (\tau\Sigma)^2 \pi_4 \left[(1-\gamma_1)(\pi_5 - \pi_2 R_\rho)(1-R_\rho)^{-1} Ri - \frac{1}{4} \alpha_3 (1-\alpha_3) \pi_4 \right] \tag{10a}$$

$$\Delta_s = 1 + (\tau\Sigma)^2 \pi_1 \left[(1-\gamma_1)(\pi_2 - \pi_3 R_\rho)(1-R_\rho)^{-1} Ri - \frac{1}{4} \alpha_3 (1-\alpha_3) \pi_1 \right] \tag{10b}$$

The coefficients π's, γ_1, α_3, and c_8, c_{11} in (12) are given at the end of Appendix A. On the other hand, the momentum fluxes $\overline{uw}, \overline{vw}$ that appear in Eqs. (8) and (9) are obtained by solving Eqs. (1a)–(1f)–(5a,b) of Appendix A, a total of seven differential equations. The buoyancy fluxes $B_{1,2}$ defined in (1g) of Appendix A are given by:

$$\begin{aligned} B_1 &= -\pi_1 \tau N^2 [\overline{uw} - (1-\alpha_3) K_\rho U_z] \\ B_2 &= -\pi_1 \tau N^2 [\overline{vw} - (1-\alpha_3) K_\rho V_z] \\ K_\rho &= (K_h - R_\rho K_s)(1-R_\rho)^{-1} \end{aligned} \tag{11a}$$

where K_ρ is the mass diffusivity, Eq. (1b) above. Since

$$\delta\rho = -\alpha_T \theta + \alpha_s s \tag{11b}$$

is invariant under $\theta \to s$, $\alpha_T \to -\alpha_s$, $R_\rho \to R_\rho^{-1}$, so are Eqs. (10a) and (10b) if:

$$\pi_1 = \pi_4, \quad \pi_3 = \pi_5 \tag{11c}$$

which coincide with the relations derived in C2.

Finally, the third-order moments in Eqs. (1a)–(1f) of Appendix A are given by Eqs. (1) of Appendix B. Contrary to the case of buoyancy dominated flows, in the case of shear dominated flows, there is no unequivocal evidence (e.g., Maurizi, 2006) in favor or against the widely used Quasi Normal Approximation (QNA) of the fourth order moments:

$$\overline{abcd} = \overline{ab}\;\overline{cd} + \overline{ac}\;\overline{bd} + \overline{ad}\;\overline{bc} \tag{11d}$$

which we shall also adopt as working hypothesis. In that case, Eqs. (1) of Appendix B yield the following TOMs:

$$2c_8\tau^{-1}\overline{w^3} = -3\overline{w^2}\frac{\partial \overline{w^2}}{\partial z} \tag{12a}$$

$$2c_8\tau^{-1}\overline{uw^2} = -\overline{uw}\frac{\partial \overline{w^2}}{\partial z} - 2\overline{w^2}\frac{\partial \overline{uw}}{\partial z} - (1-c_{11})\overline{w^3}U_z \tag{12b}$$

$$2c_8\tau^{-1}\overline{vw^2} = -\overline{vw}\frac{\partial \overline{w^2}}{\partial z} - 2\overline{w^2}\frac{\partial \overline{vw}}{\partial z} - (1-c_{11})\overline{w^3}V_z \tag{12c}$$

$$2c_8\tau^{-1}\overline{u^2w} = -\overline{w^2}\frac{\partial \overline{u^2}}{\partial z} - 2\overline{uw}\frac{\partial \overline{uw}}{\partial z} - 2(1-c_{11})\overline{uw^2}U_z \tag{12d}$$

$$2c_8\tau^{-1}\overline{v^2w} = -\overline{w^2}\frac{\partial \overline{v^2}}{\partial z} - 2\overline{vw}\frac{\partial \overline{vw}}{\partial z} - 2(1-c_{11})\overline{vw^2}V_z \tag{12e}$$

$$2c_8\tau^{-1}\overline{uvw} = -\overline{vw}\frac{\partial \overline{uw}}{\partial z} - \overline{uw}\frac{\partial \overline{vw}}{\partial z} - \overline{w^2}\frac{\partial \overline{uv}}{\partial z} - (1-c_{11})(\overline{uw^2}V_z + \overline{vw^2}U_z) \tag{12f}$$

together with:

$$\frac{\partial \varepsilon}{\partial t} + \underbrace{\frac{\partial \overline{w\varepsilon}}{\partial z}}_{\text{non-locality}} = c_1\tau^{-1}P - c_2\varepsilon\tau^{-1} \tag{12g}$$

$$P = -(\overline{uw}U_z + \overline{vw}V_z) + g\alpha_T\overline{w\theta} - g\alpha_s\overline{ws}, \quad \overline{w\varepsilon} = 0.8\tau^{-1}\left(\overline{u^2w} + \overline{v^2w} + \overline{w^3}\right) \tag{12h}$$

The non-local model for the case of shear driven flows is thus complete.

6. Convective regimes

Oceanic regimes where Deep Convection DC sets in, e.g., Labrador Sea, Gulf of Lyon and the Weddell Sea (Schott et al., 1996; Marshall and Schott, 1999; Marshall and Fiadeiro, 2002; Timmerman and Beckmann, 2003; Canuto et al., C4a), must be treated with a non-local mixing model since the eddies can be as large as the entire depth of DC. In this case, we neglect shear and treat the fluxes of T and S non-locally. Introducing the compact notation:

$$g\alpha_T\overline{w\theta} = g\alpha_T J_h \equiv B_h, \quad g\alpha_s\overline{ws} = g\alpha_s J_s \equiv B_s, \quad B = B_h - B_s$$
$$N_h^2 = g\alpha_T\frac{\partial T}{\partial z}, \quad N_s^2 = g\alpha_S\frac{\partial S}{\partial z}, \quad N^2 = N_h^2 - N_s^2 = -g\rho_0^{-1}\frac{\partial\overline{\rho}}{\partial z} = N_h^2(1-R_\rho) \tag{13a}$$

the model equations of Appendix A become:

$$\frac{\partial K}{\partial t} + \frac{\partial}{\partial z}\frac{3}{4}\overline{w^3} = B - \varepsilon \tag{13b}$$
$$\frac{\partial}{\partial t}\overline{w^2} + \underbrace{\frac{\partial\overline{w^3}}{\partial z}}_{\text{non-locality}} = \frac{2}{3}(1+2\beta_5)B - \frac{2}{3}\varepsilon - 5\tau^{-1}\left(\overline{w^2} - \frac{2K}{3}\right) \tag{13c}$$
$$\frac{\partial J_h}{\partial t} + \underbrace{\frac{\partial\overline{w^2\theta}}{\partial z}}_{\text{non-locality}} = -\overline{w^2}T_z + (1-\gamma_1)\left(g\alpha_T\overline{\theta^2} - g\alpha_s\overline{\theta s}\right) - \tau^{-1}\pi_4^{-1}J_h \tag{13d}$$
$$\frac{\partial J_s}{\partial t} + \underbrace{\frac{\partial}{\partial z}\overline{w^2 s}}_{\text{non-locality}} = -\overline{w^2}S_z + (1-\gamma_1)g\left(\alpha_T\overline{\theta s} - \alpha_s\overline{s^2}\right) - \tau^{-1}\pi_4^{-1}\overline{ws} \tag{13e}$$
$$\frac{\partial\overline{\theta^2}}{\partial t} + \underbrace{\frac{\partial}{\partial z}\overline{w\theta^2}}_{\text{non-locality}} = -2\overline{w\theta}T_z - 2\overline{\theta^2}\pi_5^{-1}\tau^{-1} \tag{13f}$$
$$\frac{\partial\overline{s^2}}{\partial t} + \underbrace{\frac{\partial}{\partial z}\overline{ws^2}}_{\text{non-locality}} = -2\overline{ws}S_z - 2\overline{s^2}\pi_5^{-1}\tau^{-1} \tag{13g}$$
$$\overline{\theta s} = -\pi_4\tau\left(\overline{ws}T_z + \overline{w\theta}S_z\right) \tag{13h}$$

together with Eqs. (12g) and (12h) for a total of seven dynamic equations like in the shear driven case. The third-order moments are taken to be the steady state solutions of Eqs. (2a)–(2c) of Appendix B, which, using the forth-order moments discussed in Appendix C, become (Cheng et al., 2005):

$$\overline{w^3} = -A_1\frac{\partial}{\partial z}\overline{w^2} - A_2\frac{\partial}{\partial z}\overline{w\theta} - A_3\frac{\partial}{\partial z}\overline{\theta^2} \tag{14a}$$
$$\overline{w^2\theta} = -A_4\frac{\partial}{\partial z}\overline{w^2} - A_5\frac{\partial}{\partial z}\overline{w\theta} - A_6\frac{\partial}{\partial z}\overline{\theta^2} \tag{14b}$$
$$\overline{w\theta^2} = -A_7\frac{\partial}{\partial z}\overline{w\theta} - A_8\frac{\partial}{\partial z}\overline{\theta^2} \tag{14c}$$

All the third-order moments exhibit a linear combination of the z-derivatives of the second-order moments, as first discussed in Canuto et al. (1994). In (14a–c), the "diffusivities" A's are given by ($\lambda = (1-c_{11})g\alpha_T$):

$$A_1 = \left(a_1\overline{w^2} + a_2\lambda\tau\overline{w\theta}\right)\tau, \quad A_2 = \left(a_3\overline{w^2} + a_4\lambda\tau\overline{w\theta}\right)\lambda\tau^2$$
$$A_3 = \left(a_5\overline{w^2} + a_6\lambda\tau\overline{w\theta}\right)\lambda^2\tau^3, \quad A_4 = a_7\tau\overline{w\theta}$$
$$A_5 = \left(a_8\overline{w^2} + a_9\lambda\tau\overline{w\theta}\right)\tau, \quad A_6 = \left(a_{10}\overline{w^2} + a_{11}\lambda\tau\overline{w\theta}\right)\lambda\tau^2$$
$$A_7 = a_{12}\tau\overline{w\theta}, \quad A_8 = \left(a_{13}\overline{w^2} + a_{14}\lambda\tau\overline{w\theta}\right)\tau \tag{14d}$$

The coefficients a_k's in (14d) are listed in Table 1.

Even though Eqs. (14a)–(14d) are relatively simple and have been successfully tested against LES data (Cheng et al., 2005), more recently we have succeeded in reducing them even further without deteriorating the comparison with LES data. In fact, we have found the following simplified version of (14a)–(14d):

$$\overline{w^3} = -0.06g\alpha\tau^2\overline{w^2}\frac{\partial\overline{w\theta}}{\partial z}, \quad \overline{w^2\theta} = -0.3\tau\overline{w^2}\frac{\partial\overline{w\theta}}{\partial z}, \quad \overline{w\theta^2} = -\tau\overline{w\theta}\frac{\partial\overline{w\theta}}{\partial z} \tag{14e}$$

Table 1
Constants in Eqs. (14d)

a_1	2.1429×10^{-1}	a_6	6.9573×10^{-4}	a_{11}	3.2468×10^{-3}
a_2	1.5306×10^{-2}	a_7	7.1429×10^{-2}	a_{12}	1.6667×10^{-1}
a_3	3.0612×10^{-2}	a_8	1.4286×10^{-1}	a_{13}	8.3333×10^{-2}
a_4	5.1020×10^{-3}	a_9	2.3810×10^{-2}	a_{14}	2.2727×10^{-2}
a_5	2.5510×10^{-3}	a_{10}	1.1905×10^{-2}		

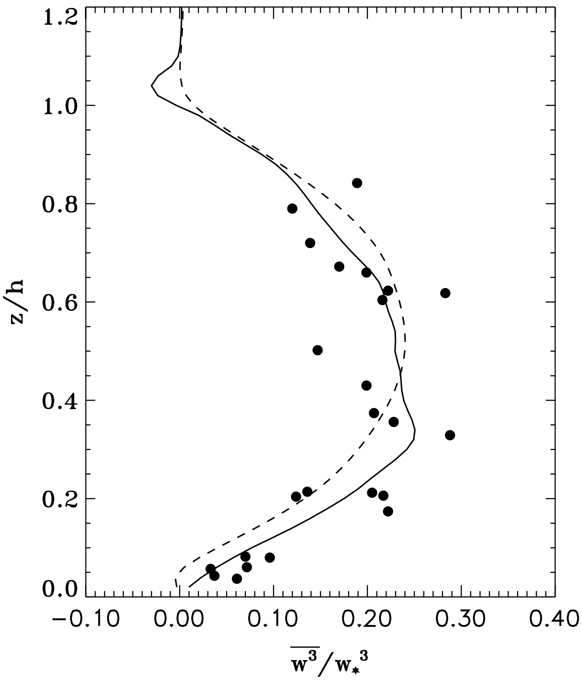

Fig. 1. The third moment $\overline{w^3}$ vs. height normalized by the PBL depth, h. The filled circles represent the aircraft data of Hartmann et al. (1999). The dashed line represents the LES data of Mironov et al. (2000). The solid line represents the result of the new model, Eq. (14e), using the second-order moments from the same LES data as input. The normalization is the Deardorff's standard normalization, $w_* = (g\alpha h\overline{w\theta}|_{\rm surf})^{1/3}$, $\theta_* = w_*^{-1}\overline{w\theta}|_{\rm surf}$.

which in Figs. 1–3 we compare with the LES data (Mironov et al., 2000) and with aircraft data (Hartmann et al., 1999). The data are reproduced quite well. The first of (14e) correctly yields a negative skewness below the cooling ocean surface (or equivalently below the cloud top in the PBL case, see Stevens et al., 2005) where $\partial B/\partial z > 0$, while it yields a positive skewness near a surface heated from below where $\partial B/\partial z < 0$. By contrast, a down-gradient type of approximation which corresponds to the first term (14a):

$$\overline{w^3} \approx -\tau\overline{w^2}\frac{\partial\overline{w^2}}{\partial z} \tag{14f}$$

would yield the wrong sign of the skewness in both the above cases. To further highlight the physical content of (14e), we can write that:

$$g\alpha\overline{w^2\theta} = 5\tau^{-1}(\overline{w^2})^{3/2}S_w, \quad g\alpha\overline{w\theta^2} = 17\tau^{-1}\overline{w\theta}(\overline{w^2})^{1/2}S_w \tag{14g}$$

which shows the role of the skewness $S_w = \overline{w^3}/(\overline{w^2})^{3/2}$, as emphasized by previous authors (Wyngaard and Weil, 1991; Hamba, 1995).

7. Plume models, old and new

Due to its importance in the formation of Atlantic deep waters, the Deep Convection regime has been extensively studied with a non-local model, specifically a plume model, that, at first sight is different from

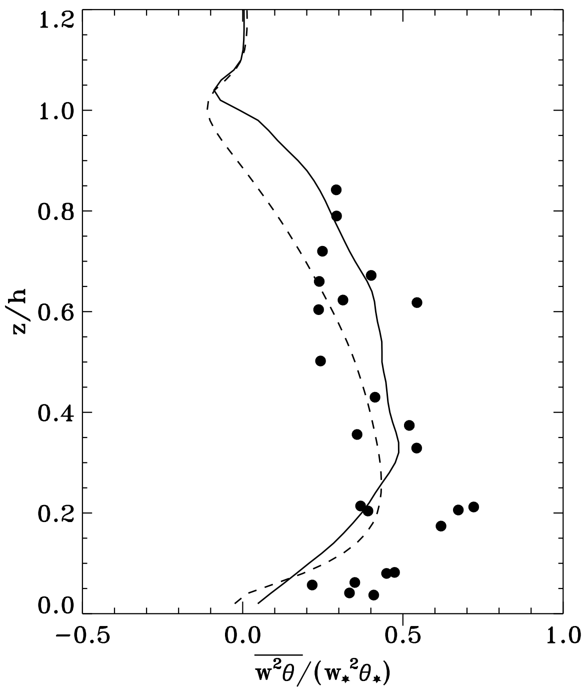

Fig. 2. Same as Fig. 1 but for $\overline{w^2\theta}$ normalized with $w_*^2\theta_*$.

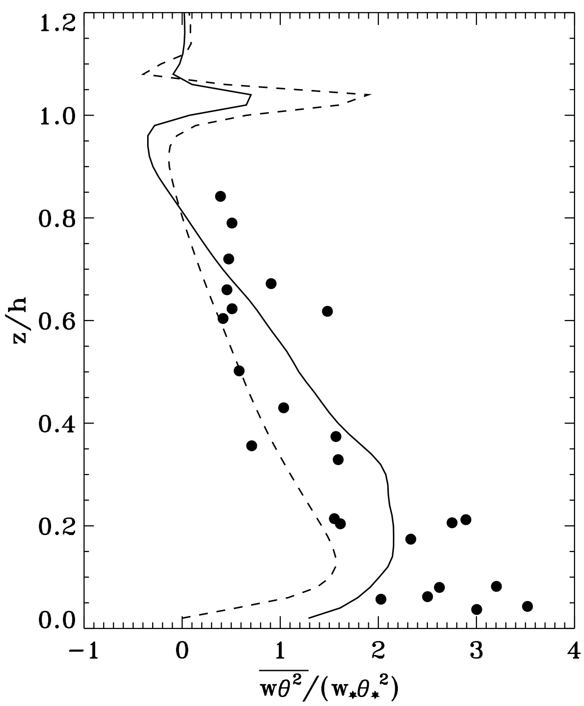

Fig. 3. Same as Fig. 1 but for $\overline{w\theta^2}$ normalized with $w_*\theta_*^2$.

the turbulence-based model we have just presented. It is therefore important to discuss the relationship between the turbulence-based model and the plume model. That is the goal of this section.

Paluszkiewicz et al. (1994), Alves (1995) and Paluszkiewicz and Romea (1997) studied Deep Convection using the only plume model available, the MTT plume model (Morton et al., 1956; Turner, 1973, 1986) which in turn was based on an original suggestion by Taylor (1945).

Plume models are attractive since they provide a rather intuitive visualization of the DC process exhibited by LES studies which show the existence of narrow descending plumes and of wide ascending plumes (the environment). Contrary to a non-local turbulence-based model that, as we have seen, is both advective and diffusive (Section 2), the MTT model is only *advective* (see Eq. (17b) below). It contains two equations representing conservation of momentum and buoyancy, Eq. (17a). However, since there are three unknowns, the third being the fraction of space occupied by the plumes that varies with z (or the plume's radius), Taylor suggested a phenomenological "*entrainment equation*" which contains an entrainment parameter α that the MTT is unable to determine. The parameter α has therefore been traditionally treated as an adjustable coefficient but in reality is a function of the large scale features of the flow. Ellison and Turner (1959) used laboratory data to determine $\alpha = \alpha(Ri)$, where Ri is the Richardson number, but this function provides a poor fit to the Mediterranean outflow data (Price and Baringer, 1994; Price and Yang, 1998). A more complete formulation of α that includes double-diffusion processes and which leads to a better representation of the data has recently been suggested (Canuto et al., 2005b). A second problem with the MTT is that it assumes that σ, the fractional area occupied by a plume, is much smaller than unity:

$$\sigma << 1, \quad \sigma = \Sigma^p(\Sigma^p + \Sigma^e)^{-1} \tag{15a}$$

where $\Sigma^p(\Sigma^e)$ is the total cross-section of the plumes (environment) at a given depth. However, since during the plume's evolution, the plumes entrain fluid from the environment, σ is bound to increase with depth to the point where (15a) becomes invalid. Specifically, *entrainment* causes the plume's mass flux $w_p\Sigma^p \propto \sigma w_p$ to increase while stable stratification decreases w_p, the net result being an increase of σ to the point where (15a) is no longer applicable. In addition, a small σ model cannot satisfy the *zero mass flux relation* ($w_{u,d}$ are the velocities of the up and down drafts and z is considered upward):

$$\sigma w_d + (1-\sigma)w_u = 0 \tag{15b}$$

which is satisfied in oceanic DC since there is no external mass flux. In addition, in the limit of small σ, Eq. (15b) implies that:

$$|w_d| >> w_u \tag{15c}$$

On the other hand, for the argument given above, when $\sigma = 1/2$, Eq. (15b) implies that:

$$w_u = |w_d| \tag{15d}$$

which is not allowed under (15a). Finally, the mass conservation (15b) is invariant under the transformation:

$$w_u \to w_d, \quad \sigma \to 1-\sigma \tag{15e}$$

and so should be any plume model. The MTT model is not invariant under (15e), and is valid only in the plumes' early development stages when the fraction of space occupied by the plumes is still small.

In summary, standard MTT plume model has the advantage of simplicity but at present: (1) it is restricted by Eq. (15a), (2) it depends on the undetermined rate of entrainment α, (3) it is only advective and it leaves out diffusion. In Table 2, we sketch the main features of the initial ($t = 0$) and final stages ($t = \infty$) of a DC event ($S_w = \overline{w^3}/(\overline{w^2})^{3/2}$).

In the fourth column we have indicated the up/down interplay. In the early stages, the downdrafts dominate over updrafts, while in the final stages, updrafts and downdrafts are equally important. The last two

Table 2
Deep convection

Time	S_w	σ	Up/down	Diff	Adv
Initial phase	<0	Small	$\|w_d\| >> w_u$	No	Yes
Final phase	≈0	1/2	$w_u \approx \|w_d\|$	Yes	No

columns show that the initial stages are governed by advection while the final stages are governed by diffusion. To correct the limitations of the MTT model, we proceed as follows:

(1) We use the turbulence-based mixing model and limit the non-locality to the heat and salinity fluxes.
(2) The new plume model, being turbulence based, is such that all relations are invariant under (15e) and thus the model is valid throughout the entire plume's development.
(3) As a basic simplifying assumption, we write the non-local TOMs in the "plume approximation" which assumes a top hat profile that consists of two delta functions for the pdf of each state variable, corresponding to ascending and descending plumes. This implies (Lappen and Randall, 2001) that such a profile has 100% probability of having one of just two possible values, the two allowed states being up-drafts and down-drafts. This introduces a considerable simplification to the problem since it reduces substantially the number of higher-order moments that are needed, it assures the realizability condition of the higher order moments and requires fewer prognostic equations.

8. New plume model

To "*plumenize*" the TOMs using the up-down draft notation, we first employ the following relations (Canuto and Dubovikov, 1998):

$$\overline{w^2} = \sigma(1-\sigma)(w_u - w_d)^2 = \beta_\sigma w^2, \quad \beta_\sigma = \sigma(1-\sigma)^{-1} \tag{16a}$$
$$J_h = \sigma(1-\sigma)(w_u - w_d)(\theta_u - \theta_d) \tag{16b}$$
$$\overline{\theta^2} = \sigma(1-\sigma)(\theta_u - \theta_d)^2 = \beta_\sigma^{-1} w^{-2} J_h^2 \tag{16c}$$

where $w \equiv w_d$. Analogous relations hold for the salinity field. These relations are invariant under (15e). Thus, the plumenized TOMs become:

$$\begin{aligned}
\overline{w^3} &= -\sigma(1-\sigma)(1-2\sigma)(w_u - w_d)^3 = (\overline{w^2})^{3/2} S_w \\
\overline{w^2\theta} &= -\sigma(1-\sigma)(1-2\sigma)(\theta_u - \theta_d)(w_u - w_d)^2 = (\overline{w^2})^{1/2} S_w J_h \\
\overline{w\theta^2} &= -\sigma(1-\sigma)(1-2\sigma)(\theta_u - \theta_d)^2(w_u - w_d) = S_\theta J_h (\overline{\theta^2})^{1/2} \\
\overline{w^2 s} &= (\overline{w^2})^{1/2} S_w J_s \\
\overline{ws^2} &= S_s J_s (\overline{s^2})^{1/2}
\end{aligned} \tag{16d}$$

where the skewness of any field is taken to be:

$$S_a \equiv (2\sigma - 1)[\sigma(1-\sigma)]^{-1/2} \tag{16e}$$

In conclusion, the complete new plume model is given by Eqs. (13a)–(13h), (16d), (16e).

9. The small σ limit. The MTT model

The goal of this section is to prove that the plume model just derived, which is valid for any σ, contains the MTT in the limit for small σ. That is the goal of this section. The MTT model contains three equations representing the plume's kinetic energy $1/2w^2$, the fractional area σ occupied by the plume and the buoyancy $B(\text{cm}^2\,\text{s}^{-3})$. They are (Turner, 1973; Eqs. 6.1.4 with $b^2 = \sigma\ell^2$ and for rising plumes with z pointing upward, $w > 0$):

$$\begin{aligned}
\frac{\partial w^2}{\partial z} &= \frac{2B}{\sigma w} - \frac{4\alpha}{\ell}\frac{w^2}{\sigma^{1/2}} \\
\frac{\partial \sigma}{\partial z} &= -\frac{B}{w^3} + \frac{4\alpha\sigma^{1/2}}{\ell} \\
\frac{\partial B}{\partial z} &= -\sigma w \mathrm{N}^2, \quad \mathrm{N}^2 \equiv -g\rho_{\text{ref}}^{-1}\,\mathrm{d}\rho_{env}/\mathrm{d}z
\end{aligned} \tag{17a}$$

where α is the entrainment coefficient discussed earlier, the subscript "env" stands for environment and "ref" stands for a reference density in the environment. Eqs. (17a) are not invariant under (15e) since they are only applicable in the regime (15a). If one substitutes the buoyancy equation into the mean temperature equation, one obtains:

$$\frac{\partial T}{\partial t} + (\overline{w} + w_{\text{adv}})\frac{\partial T}{\partial z} = 0, \quad w_{\text{adv}} = -\sigma w \tag{17b}$$

Since the rhs of the first of (17b) is zero, there is no diffusion which shows what we stated earlier that the MTT is solely advective with an advection velocity w_{adv} that is σ times the plume's velocity. An additional interesting variable is the plume's "mass flux" defined as:

$$M = \sigma w \tag{17c}$$

Using (17a), one obtains the relation:

$$M^{-1}\frac{\partial M}{\partial z} = E - D = \frac{2\alpha}{\ell}\sigma^{-1/2} > 0 \tag{17d}$$

where E and D stand for the rates of entrainment and detrainment respectively. Since the rhs of (17d) is positive, MTT *accounts only for entrainment but not detrainment* which is understandable since detrainment requires a dynamical environment which is excluded in the MTT model which assumes the environment to be quiescent.

In the ocean case ($w < 0$) and the small σ limit, we have from Eqs. (16a)–(16e) that:

$$\beta_\sigma = \sigma, \quad S_w = -\sigma^{-1/2}, \quad \overline{w^2} = \sigma w^2 \tag{18a}$$

and thus from Eq. (16d) it follows that:

$$\overline{w^3} = \sigma w^3, \quad \overline{w^2\theta} = wJ_h, \quad \overline{w^2 s} = wJ_s, \quad \overline{w\theta^2} = \sigma^{-1/2}J_h(\overline{\theta^2})^{1/2}, \quad \overline{ws^2} = \sigma^{-1/2}J_s(\overline{s^2})^{1/2} \tag{18b}$$

Using (18b), the first of Eq. (14e) becomes:

$$\frac{\partial J_h}{\partial z} = -\frac{w}{Cg\alpha\tau^2} \tag{18c}$$

Next, using (13c) and (13d), together with (18b), we obtain:

$$w^3\frac{\partial \sigma}{\partial z} + \frac{3\sigma w}{2}\frac{\partial w^2}{\partial z} = \frac{2}{3}(1+2\beta_5)B - \frac{4\sigma w^2}{\tau} \tag{18d}$$

$$w\frac{\partial J_h}{\partial z} + \frac{J_h}{2w}\frac{\partial w^2}{\partial z} = -\sigma w^2 T_z + (1-\gamma_1)g\alpha\sigma^{-1}w^{-2}J_h^2 - \tau^{-1}\pi_4^{-1}J_h \tag{18e}$$

Solving Eqs. (18c)–(18e), and using (the coefficient C_0 will be discussed later):

$$\tau = -C_0\sigma^{1/2}w^{-1}\ell \tag{18f}$$

we obtain:

$$\frac{\partial w^2}{\partial z} = 2(1-\gamma_1)w^{-1}\sigma^{-1}B + 2C_0^{-1}\pi_4^{-1}w^2\sigma^{-1/2}\ell^{-1} - 2B^{-1}w^3\sigma(N_h^2 - C^{-1}C_0^{-2}\sigma^{-2}\ell^{-2}w^2) \tag{19a}$$

$$\frac{\partial \sigma}{\partial z} = (3\gamma_1 + 4\beta_5/3 - 7/3)Bw^{-3} + (C_0\pi_4)^{-1}(4\pi_4 - 3)\sigma^{1/2}\ell^{-1} + 3wB^{-1}(\sigma^2 N_h^2 - C^{-1}C_0^{-2}w^2\ell^{-2}) \tag{19b}$$

Using the values:

$$C = 0.06, \quad \beta_5 = 1/2, \quad \gamma_1 = 1/3, \quad \pi_4 = 0.08372 \tag{19c}$$

Eqs. (18d) and (18e) become:

$$\frac{\partial w^2}{\partial z} = 1.3w^{-1}\sigma^{-1}B + 24C_0^{-1}w^2\sigma^{-1/2}\ell^{-1} - 2B^{-1}w^3\sigma(N_h^2 - 17C_0^{-2}\sigma^{-2}\ell^{-2}w^2) \tag{19d}$$

$$\frac{\partial \sigma}{\partial z} = -0.7Bw^{-3} - 32C_0^{-1}\sigma^{1/2}\ell^{-1} + 3wB^{-1}(\sigma^2 N_h^2 - 17C_0^{-2}w^2\ell^{-2}) \tag{19e}$$

Since in our system z is positive upward, and the descending plume is small near the surface getting progressively larger at depth, $\mathrm{d}\sigma/\mathrm{d}z < 0$, the second term in the rhs of (19e) that represents entrainment, must be negative. By the same token, the second term in (19d) is positive since $\mathrm{d}w^2/\mathrm{d}z > 0$. If $C_0 = 6$ (which comes from relating the dissipation length scale in (18f) to the ℓ in Eqs. (17a)), Eqs. (19d) and (19e) compare well with Eq. (17a) of the MTT model (their Eq. 6.1.4) and Eqs. (10)–(11) of Paluszkiewicz and Romea (1997).

10. Conclusions

In this paper we have developed a non-local mixing model based on the Reynolds Stress formalism. We have presented the most general non-local model that today's knowledge in turbulent closure allowed us to formulate. Clearly, the full model in which all the fields of temperature, salinity and 3D velocities are treated non-locally, is fairly complex. To assess the validity of non-locality, we have worked out two simplified models. One is valid in Deep Convective regions and the other where strong winds release bursts of mechanical energy that is transported through the mixed layer by energetic eddies which require a non-local treatment.

The case of Deep Convection (DC) was in the past treated with the non-local model represented by the plume model (PM) of Morton et al. (1956), (MTT). Such a model has two substantial limitations, it is only advective while in the final stages of DC diffusion dominates and the rate of entrainment is treated as an adjustable quantity. By rewriting the turbulence-based mixing model developed here in the plume formalism, a new PM emerges which no longer suffers from the limitations of the MTT model and is valid for the entire development of a convective regime.

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Appendix A. Shear and buoyancy. Second-order moments

Here we present the explicit forms of the dynamic equations for the second-order moments of interest (the general equations can be found in e.g., André et al., 1982; Mellor and Yamada, 1974, 1982; and Canuto, 1992):

$$\frac{\partial}{\partial t}\overline{uw} + \underbrace{\frac{\partial}{\partial z}\overline{uw^2}}_{\text{non-locality}} = \frac{1}{2}\left[\frac{4}{5}K + (\alpha_1 - \alpha_2)\overline{u^2} + (\alpha_1 + \alpha_2 - 2)\overline{w^2}\right]U_z + \frac{1}{2}(\alpha_1 - \alpha_2)\overline{uv}V_z + \beta_5 B_1 - 2\tau_{pv}^{-1}\overline{uw} \tag{1a}$$

$$\frac{\partial}{\partial t}\overline{vw} + \underbrace{\frac{\partial}{\partial z}\overline{vw^2}}_{\text{non-locality}} = \frac{1}{2}\left[\frac{4}{5}K + (\alpha_1 - \alpha_2)\overline{v^2} + (\alpha_1 - \alpha_2 - 2)\overline{w^2}\right]V_z + \frac{1}{2}(\alpha_1 - \alpha_2)\overline{uv}U_z + \beta_5 B_2 - 2\tau_{pv}^{-1}\overline{vw} \tag{1b}$$

$$\frac{\partial}{\partial t}\overline{uv} + \underbrace{\frac{\partial}{\partial z}\overline{uvw}}_{\text{non-locality}} = -\left[1 - \frac{1}{2}(\alpha_1 + \alpha_2)\right](\overline{uw}V_z + \overline{vw}U_z) - 2\tau_{pv}^{-1}\overline{uv} \tag{1c}$$

$$\frac{\partial}{\partial t}\overline{w^2} + \underbrace{\frac{\partial}{\partial z}\overline{w^3}}_{\text{non-locality}} = \left(\frac{1}{3}\alpha_1 - \alpha_2\right)(\overline{uw}U_z + \overline{vw}V_z) + \frac{2}{3}(1 + 2\beta_5)B - \frac{2}{3}\varepsilon - 2\tau_{pv}^{-1}\left(\overline{w^2} - \frac{2K}{3}\right) \tag{1d}$$

$$\frac{\partial}{\partial t}\overline{u^2} + \underbrace{\frac{\partial}{\partial z}\overline{u^2w}}_{\text{non-locality}} = \left(\frac{1}{3}\alpha_1 + \alpha_2 - 2\right)\overline{uw}U_z - \frac{2}{3}\alpha_1\overline{vw}V_z + \frac{2}{3}(1 - \beta_5)B - \frac{2}{3}\varepsilon - 2\tau_{pv}^{-1}\left(\overline{u^2} - \frac{2K}{3}\right) \tag{1e}$$

$$\frac{\partial K}{\partial t} + \frac{1}{2}\underbrace{\frac{\partial}{\partial z}(\overline{u^2w} + \overline{v^2w} + \overline{w^3})}_{\text{non-locality}} = -(\overline{uw}U_z + \overline{vw}V_z) + B - \varepsilon \tag{1f}$$

The temperature/salinity fields enter through the fluxes $B_{1,2,3}$ defined as follows:

$$B_i = g(\alpha_T\overline{u_i\theta} - \alpha_s\overline{u_is}), \quad B_3 \equiv B = g(\alpha_T\overline{w\theta} - \alpha_s\overline{ws}) \tag{1g}$$

The dynamic equations for the following six fluxes:

$$\overline{u\theta}, \overline{v\theta}, \overline{w\theta}, \overline{us}, \overline{vs}, \overline{ws}$$

are given by:

$$\frac{\partial}{\partial t}\overline{u\theta} + \underbrace{\frac{\partial}{\partial z}\overline{uw\theta}}_{\text{non-locality}} = -\overline{uw}T_z - (1-\alpha_3)\overline{w\theta}U_z - \tau_{p\theta}^{-1}\overline{u\theta} \tag{2a}$$

$$\frac{\partial}{\partial t}\overline{v\theta} + \underbrace{\frac{\partial}{\partial z}\overline{vw\theta}}_{\text{non-locality}} = -\overline{vw}T_z - (1-\alpha_3)\overline{w\theta}V_z - \tau_{p\theta}^{-1}\overline{v\theta} \tag{2b}$$

$$\frac{\partial}{\partial t}\overline{w\theta} + \underbrace{\frac{\partial}{\partial z}\overline{w^2\theta}}_{\text{non-locality}} = -\overline{w^2}T_z + (1-\gamma_1)g\left(\alpha_T\overline{\theta^2} - \alpha_S\overline{\theta s}\right) - \frac{\alpha_3}{4}\left(\overline{u\theta}U_z + \overline{v\theta}V_z\right) - \tau_{p\theta}^{-1}\overline{w\theta} \tag{2c}$$

$$\frac{\partial}{\partial t}\overline{us} + \underbrace{\frac{\partial}{\partial z}\overline{uws}}_{\text{non-locality}} = -\overline{uw}S_z - (1-\alpha_3)\overline{ws}U_z - \tau_{ps}^{-1}\overline{us} \tag{3a}$$

$$\frac{\partial}{\partial t}\overline{vs} + \underbrace{\frac{\partial}{\partial z}\overline{vws}}_{\text{non-locality}} = -\overline{vw}S_z - (1-\alpha_3)\overline{ws}V_z - \tau_{ps}^{-1}\overline{vs} \tag{3b}$$

$$\frac{\partial}{\partial t}\overline{ws} + \underbrace{\frac{\partial}{\partial z}\overline{w^2s}}_{\text{non-locality}} = -\overline{w^2}S_z + (1-\gamma_1)g\left(\alpha_T\overline{\theta s} - \alpha_s\overline{s^2}\right) - \frac{\alpha_3}{4}\left(\overline{us}U_z + \overline{vs}V_z\right) - \tau_{ps}^{-1}\overline{ws} \tag{3c}$$

The temperature and salinity variances satisfy the dynamic equations:

$$\frac{\partial\overline{\theta^2}}{\partial t} + \underbrace{\frac{\partial}{\partial z}\overline{w\theta^2}}_{\text{non-locality}} = -2\overline{w\theta}T_z - 2\overline{\theta^2}\tau_\theta^{-1} \tag{4a}$$

$$\frac{\partial\overline{s^2}}{\partial t} + \underbrace{\frac{\partial}{\partial z}\overline{ws^2}}_{\text{non-locality}} = -2\overline{ws}S_z - 2\overline{s^2}\tau_s^{-1} \tag{4b}$$

The temperature–salinity correlation is taken to be (C2, Eq. (11)):

$$\overline{\theta s} = -\tau_{s\theta}(\overline{ws}T_z + \overline{w\theta}S_z) \tag{4c}$$

Finally, the dynamic equation for the dissipation rate ε is given by Canuto et al. (1994):

$$\frac{\partial\varepsilon}{\partial t} + \underbrace{\frac{\partial\overline{w\varepsilon}}{\partial z}}_{\text{non-locality}} = c_1\tau^{-1}(-\overline{u_iu_j}U_{i,j} + B) - c_2\varepsilon\tau^{-1} \tag{5a}$$

with:

$$\overline{w\varepsilon} = 0.8\tau^{-1}(\overline{u^2w} + \overline{v^2w} + \overline{w^3}), \quad c_1 = 2.88, \quad c_2 = 3.84 \tag{5b}$$

Furthermore ($Ko = 1.66$ is the Kolmogorov constant):

$$\begin{aligned} &\tau_{pv} = \frac{2}{5}\tau, \quad \tau_{p\theta} = \tau_{ps} = \pi_1\tau = \pi_4\tau, \quad \pi_1 = \left(\frac{27}{5}Ko^3\right)^{-1/2}(1+\sigma_t^{-1})^{-1} \\ &\tau_\theta = \tau_s = \pi_3\tau = \pi_5\tau, \quad \pi_3 = \sigma_t = 0.72, \quad \tau_{s\theta} = \frac{1}{3}\tau, \quad \beta_5 = \frac{1}{2} \end{aligned} \tag{5c}$$

$$\alpha_3 = 0.29,\ \gamma_1 = 1/3,\ c_8 = 5,\ c_{11} = 0.1 \tag{5d}$$
$$\tau = 2K/\varepsilon \tag{5e}$$

We have a total of 15 differential equations.

Appendix B. Shear and buoyancy. Third-order moments

B.1. Velocity field

$$\frac{\partial}{\partial t}\overline{w^3} = -\frac{\partial}{\partial z}\overline{w^4} + 3\overline{w^2}\frac{\partial\overline{w^2}}{\partial z} - 2c_8\tau^{-1}\overline{w^3} + 3(1-c_{11})g\alpha\overline{w^2\theta} \tag{1a}$$
$$\frac{\partial}{\partial t}\overline{uw^2} = -\frac{\partial}{\partial z}\overline{uw^3} - (1-c_{11})\overline{w^3}U_z + 2\overline{uw}\frac{\partial\overline{w^2}}{\partial z} + \overline{w^2}\frac{\partial\overline{uw}}{\partial z} - 2c_8\tau^{-1}\overline{uw^2} + 2(1-c_{11})g\alpha\overline{uw\theta} \tag{1b}$$
$$\frac{\partial}{\partial t}\overline{vw^2} = -\frac{\partial}{\partial z}\overline{vw^3} - (1-c_{11})\overline{w^3}V_z + 2\overline{vw}\frac{\partial\overline{w^2}}{\partial z} + \overline{w^2}\frac{\partial\overline{vw}}{\partial z} - 2c_8\tau^{-1}\overline{vw^2} + 2(1-c_{11})g\alpha\overline{vw\theta} \tag{1c}$$
$$\frac{\partial}{\partial t}\overline{u^2w} = -\frac{\partial}{\partial z}\overline{u^2w^2} - 2(1-c_{11})\overline{uw^2}U_z + \overline{u^2}\frac{\partial\overline{w^2}}{\partial z} + 2\overline{uw}\frac{\partial\overline{uw}}{\partial z} - 2c_8\tau^{-1}\overline{u^2w} + (1-c_{11})g\alpha\overline{u^2\theta} \tag{1d}$$
$$\frac{\partial}{\partial t}\overline{v^2w} = -\frac{\partial}{\partial z}\overline{v^2w^2} - 2(1-c_{11})\overline{vw^2}V_z + \overline{v^2}\frac{\partial\overline{w^2}}{\partial z} + 2\overline{vw}\frac{\partial\overline{vw}}{\partial z} - 2c_8\tau^{-1}\overline{v^2w} + (1-c_{11})g\alpha\overline{v^2\theta} \tag{1e}$$
$$\begin{aligned}\frac{\partial}{\partial t}\overline{uvw} = &-\frac{\partial}{\partial z}\overline{uvw^2} - (1-c_{11})\left(\overline{uw^2}V_z + \overline{vw^2}U_z\right) + \overline{uv}\frac{\partial\overline{w^2}}{\partial z} + \overline{uw}\frac{\partial\overline{vw}}{\partial z} + \overline{vw}\frac{\partial\overline{uw}}{\partial z}\\ &- 2c_8\tau^{-1}\overline{uvw} + (1-c_{11})g\alpha\overline{uv\theta}\end{aligned} \tag{1f}$$

B.2. Temperature field

$$\frac{\partial}{\partial t}\overline{w^2\theta} = -\frac{\partial}{\partial z}\overline{w^3\theta} + \overline{w^2}\frac{\partial\overline{w\theta}}{\partial z} + 2\overline{w\theta}\frac{\partial\overline{w^2}}{\partial z} - \overline{w^3}T_z - 2c_8\tau^{-1}\overline{w^2\theta} + 2(1-c_{11})g\alpha\overline{w\theta^2} \tag{2a}$$
$$\frac{\partial}{\partial t}\overline{w\theta^2} = -\frac{\partial}{\partial z}\overline{w^2\theta^2} + 2\overline{w\theta}\frac{\partial\overline{w\theta}}{\partial z} + \overline{\theta^2}\frac{\partial\overline{w^2}}{\partial z} - 2\overline{w^2\theta}T_z - 2c_8\tau^{-1}\overline{w\theta^2} + (1-c_{11})g\alpha\overline{\theta^3} \tag{2b}$$
$$\frac{\partial}{\partial t}\overline{\theta^3} = -\frac{\partial\overline{w\theta^3}}{\partial z} + 3\overline{\theta^2}\frac{\partial\overline{w\theta}}{\partial z} - 3\overline{w\theta^2}T_z - 2c_{10}\tau^{-1}\overline{\theta^3} \tag{2c}$$
$$\frac{\partial}{\partial t}\overline{u\theta^2} = -\frac{\partial}{\partial z}\overline{uw\theta^2} - (1-c_{11})\overline{w\theta^2}U_z + 2\overline{u\theta}\frac{\partial\overline{w\theta}}{\partial z} + \overline{\theta^2}\frac{\partial\overline{uw}}{\partial z} - 2\overline{uw\theta}T_z - 2c_8\tau^{-1}\overline{u\theta^2} \tag{2d}$$
$$\frac{\partial}{\partial t}\overline{v\theta^2} = -\frac{\partial}{\partial z}\overline{vw\theta^2} - (1-c_{11})\overline{w\theta^2}V_z + 2\overline{v\theta}\frac{\partial\overline{w\theta}}{\partial z} + \overline{\theta^2}\frac{\partial\overline{vw}}{\partial z} - 2\overline{vw\theta}T_z - 2c_8\tau^{-1}\overline{v\theta^2} \tag{2e}$$
$$\begin{aligned}\frac{\partial}{\partial t}\overline{uw\theta} = &-\frac{\partial}{\partial z}\overline{uw^2\theta} - (1-c_{11})\overline{w^2\theta}U_z + \overline{uw}\frac{\partial\overline{w\theta}}{\partial z} + \overline{u\theta}\frac{\partial\overline{w^2}}{\partial z} + \overline{w\theta}\frac{\partial\overline{uw}}{\partial z} - \overline{uw^2}T_z - 2c_8\tau^{-1}\overline{uw\theta}\\ &+ (1-c_{11})g\alpha\overline{u\theta^2}\end{aligned} \tag{2f}$$
$$\begin{aligned}\frac{\partial}{\partial t}\overline{vw\theta} = &-\frac{\partial}{\partial z}\overline{vw^2\theta} - (1-c_{11})\overline{w^2\theta}V_z + \overline{vw}\frac{\partial\overline{w\theta}}{\partial z} + \overline{v\theta}\frac{\partial\overline{w^2}}{\partial z} + \overline{w\theta}\frac{\partial\overline{vw}}{\partial z} - \overline{vw^2}T_z - 2c_8\tau^{-1}\overline{vw\theta}\\ &+ (1-c_{11})g\alpha\overline{v\theta^2}\end{aligned} \tag{2g}$$
$$\frac{\partial}{\partial t}\overline{u^2\theta} = -\frac{\partial}{\partial z}\overline{u^2w\theta} - 2(1-c_{11})\overline{uw\theta}U_z + \overline{u^2}\frac{\partial\overline{w\theta}}{\partial z} + 2\overline{u\theta}\frac{\partial\overline{uw}}{\partial z} - \overline{u^2w}T_z - 2c_8\tau^{-1}\overline{u^2\theta} \tag{2h}$$
$$\frac{\partial}{\partial t}\overline{v^2\theta} = -\frac{\partial}{\partial z}\overline{v^2w\theta} - 2(1-c_{11})\overline{vw\theta}V_z + \overline{v^2}\frac{\partial\overline{w\theta}}{\partial z} + 2\overline{v\theta}\frac{\partial\overline{vw}}{\partial z} - \overline{v^2w}T_z - 2c_8\tau^{-1}\overline{v^2\theta} \tag{2i}$$
$$\frac{\partial}{\partial t}\overline{uv\theta} = -\frac{\partial}{\partial z}\overline{uvw\theta} - (1-c_{11})\left(\overline{uw\theta}V_z + \overline{vw\theta}U_z\right) + \overline{uv}\frac{\partial\overline{w\theta}}{\partial z} + \overline{u\theta}\frac{\partial\overline{vw}}{\partial z} + \overline{v\theta}\frac{\partial\overline{uw}}{\partial z} - \overline{uvw}T_z - 2c_8\tau^{-1}\overline{uv\theta} \tag{2j}$$

Appendix C. Fourth-order moments

C.1. Previous models

Most previous models (Tatsumi, 1957; O'Brien and Francis, 1962; Ogura, 1962; Zeman and Lumley, 1976; André et al., 1976, 1978; Bougeault, 1981; Chen and Cotton, 1983; Moeng and Randall, 1984; Canuto et al., 1994) employed the quasi-normal approximation, QNA, Eq. (11d). As discussed in detail in Cheng et al. (2005), in the case of the temperature field, Eq. (11d) can cause violations of the realizability condition derived from Schwarz' generalized inequalities (André et al., 1976):

$$|\overline{abc}| \leqslant \min \left\{ \begin{array}{l} [\overline{a^2}(\overline{b^2}\,\overline{c^2} + \overline{bc}^2)]^{\frac{1}{2}} \\ [\overline{b^2}(\overline{a^2}\,\overline{c^2} + \overline{ac}^2)]^{\frac{1}{2}} \\ [\overline{c^2}(\overline{a^2}\,\overline{b^2} + \overline{ab}^2)]^{\frac{1}{2}} \end{array} \right\} \tag{1a}$$

where a, b, and c stand for any of u, v, w and θ. In the stable case, Moeng and Randall (1984) pointed out that QNA leads to a "wave equation" for the third-order moment:

$$\frac{\partial^2}{\partial t^2}\overline{w^3} = -3g\alpha\overline{w^3}\frac{\partial T}{\partial z} + \text{other terms} \tag{1b}$$

with an oscillation frequency of $f = (3g\alpha\partial T/\partial z)^{1/2}$. Similar "wave equations" resulted from other TOM equations. The oscillations generated by these "wave equations" occur in the numerical simulations but are not observed in the PBL and thus are spurious.

C.2. New model (Cheng et al., 2005; cited a C5)

Since the QNA neglects the cumulants, the new model must account for them. In principle, to formulate a new model for the FOMs (fourth-order moments), one could begin with the dynamic equations of the FOMs, but this would bring about a new set of parameterizations for the pressure and dissipation terms, and most of all, the need to model the fifth-order moments. C5 proposed a new and simpler approach. Using as an input the LES data for second and third-order moments, they derived information about the fourth-order cumulants. To proceed, they re-wrote the third-order moment equations by subtracting from both sides the QNA expressions (11d). The results are ($\lambda = (1 - c_{11})g\alpha$, $\beta = -\partial T/\partial z$):

$$\frac{\partial}{\partial z}\left(\overline{w^4} - \overline{w^4}|_{QN}\right) = -2c_8\frac{\overline{w^3}}{\tau} + 3\lambda\overline{w^2\theta} - 3\overline{w^2}\frac{\partial}{\partial z}\overline{w^2} \tag{2a}$$

$$\frac{\partial}{\partial z}\left(\overline{w^3\theta} - \overline{w^3\theta}|_{QN}\right) = -2c_8\frac{\overline{w^2\theta}}{\tau} + \beta\overline{w^3} + 2\lambda\overline{w\theta^2} - 2\overline{w^2}\frac{\partial}{\partial z}\overline{w\theta} - \overline{w\theta}\frac{\partial}{\partial z}\overline{w^2} \tag{2b}$$

$$\frac{\partial}{\partial z}\left(\overline{w^2\theta^2} - \overline{w^2\theta^2}|_{QN}\right) = -2c_8\frac{\overline{w\theta^2}}{\tau} + 2\beta\overline{w^2\theta} + \lambda\overline{\theta^3} - \overline{w^2}\frac{\partial}{\partial z}\overline{\theta^2} - 2\overline{w\theta}\frac{\partial}{\partial z}\overline{w\theta} \tag{2c}$$

$$\frac{\partial}{\partial z}\left(\overline{w\theta^3} - \overline{w\theta^3}|_{QN}\right) = -2c_{10}\frac{\overline{\theta^3}}{\tau} + 3\beta\overline{w\theta^2} - 3\overline{w\theta}\frac{\partial}{\partial z}\overline{\theta^2} \tag{2d}$$

$$\frac{\partial}{\partial z}\left(\overline{u^2w^2} - \overline{u^2w^2}|_{QN}\right) = -2c_8\frac{\overline{u^2w}}{\tau} + \lambda\overline{u^2\theta} - \overline{w^2}\frac{\partial\overline{u^2}}{\partial z} \tag{2e}$$

$$\frac{\partial}{\partial z}\left(\overline{u^2w\theta} - \overline{u^2w\theta}|_{QN}\right) = -2c_8\frac{\overline{u^2\theta}}{\tau} + \beta\overline{u^2w} - \overline{w\theta}\frac{\partial\overline{u^2}}{\partial z} \tag{2f}$$

The lhs represent the z-derivatives of the cumulants that were parameterized as follows. Use of LES data to estimate the rhs of Eq. (2) led C5 to conclude that a good representation is as follows:

$$\frac{\partial}{\partial z}\left(\overline{w^4}-\overline{w^4}|_{QN}\right)=p_1\frac{\overline{w^3}}{\tau},\quad \frac{\partial}{\partial z}\left(\overline{w^3\theta}-\overline{w^3\theta}|_{QN}\right)=p_2\frac{\overline{w^2\theta}}{\tau}+d_1\beta\overline{w^3} \tag{3a}$$

$$\frac{\partial}{\partial z}\left(\overline{w^2\theta^2}-\overline{w^2\theta^2}|_{QN}\right)=p_3\frac{\overline{w\theta^2}}{\tau}+d_2\beta\overline{w^2\theta},\quad \frac{\partial}{\partial z}\left(\overline{w\theta^3}-\overline{w\theta^3}|_{QN}\right)=p_4\frac{\overline{\theta^3}}{\tau}+d_3\beta\overline{w\theta^2} \tag{3b}$$

$$\frac{\partial}{\partial z}\left(\overline{u^2w^2}-\overline{u^2w^2}|_{QN}\right)=p_5\frac{\overline{u^2w}}{\tau},\quad \frac{\partial}{\partial z}\left(\overline{u^2w\theta}-\overline{u^2w\theta}|_{QN}\right)=p_6\frac{\overline{u^2\theta}}{\tau}+d_4\beta\overline{u^2w} \tag{3c}$$

The constants p's and d's were then chosen so that (3a)–(3c) best match the full expressions (2a)–(2f) using as input the LES data for the TOMs and SOMs (second-order moments) (Mironov et al., 2000). A key role was played by the aircraft data by Hartmann et al. (1999). The "best" values were chosen as whole numbers for simplicity and are listed in Table 1 of C5 who also plotted the z-derivatives of the cumulants (their Fig. 1). These figures show that Eqs. (3) is a better approximation than that of previous authors (Gryanik and Hartmann, 2002).

The choice of the constants p's by C5 effectively modifies the coefficients of the slow terms in the TOM equations, and thus provides adequate damping that was lacking in previous models. In addition, the choice of the constants d's makes the z-derivatives of the cumulants cancel out the β terms in the TOM equations, as Eqs. (14) of the text show. While Zeman and Lumley (1976) also neglected β in some of the TOM equations arguing that they are small, C5 argued that the β terms are canceled by the non-zero cumulants. This argument is supported by the TOM equations and the LES data presented in Fig. 1 of C5. In addition, the cancellation of the β terms not only greatly simplifies the TOM equations, but also avoids the singularities in the unstable case and eliminates the source of the spurious oscillations in the stable case discussed above.

To assess the validity of the new FOM model, C5 compared (3) with the measured data by plotting the modeled FOMs with the SOMs and TOMs from the LES data (Mironov et al., 2000) as input, versus z/h (h is the PBL height). Also plotted in C5 are the aircraft data of Hartmann et al. (1999), the model results of Gryanik and Hartmann, 2002) and QNA respectively. The kurtosis of w from the models and from the aircraft data is plotted in Fig. 2e of C5. To help assess the improvement shown in Fig. 2e, we refer the reader to the measurements of w-kurtosis by Lenschow et al. (1994, 2000), who stated that "The kurtosis increases with height from around 3 to about 5 near 0.9 z/z_i. Above $0.9z/z_i$ the kurtosis increases sharply". In Fig. 2f, C5 plotted the w-kurtosis K_w versus skewness S_w from the new model and from Gryanik and Hartmann (2002) to be compared with the aircraft data and with the empirical formula (Alberighi et al., 2002)

$$K_w = 2.3(S_w^2+1) \tag{3d}$$

Judging from the comparisons with these data, the new model exhibits significant improvements when compared with the QNA and with the Gryanik and Hartmann (2002) model.

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